Frank NoÃ©

List of Publications by Year
in descending order

149 papers	15,875 citations	23567 58 h-index	19190 118 g-index
170 all docs	**170** docs citations	**170** times ranked	**10066** citing authors

#	Article	IF	Citations
1	Markov models of molecular kinetics: Generation and validation. Journal of Chemical Physics, 2011, 134, 174105.	3.0	968
2	PyEMMA 2: A Software Package for Estimation, Validation, and Analysis of Markov Models. Journal of Chemical Theory and Computation, 2015, 11, 5525-5542.	5.3	876
3	Identification of slow molecular order parameters for Markov model construction. Journal of Chemical Physics, 2013, 139, 015102.	3.0	777
4	Constructing the equilibrium ensemble of folding pathways from short off-equilibrium simulations. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 19011-19016.	7.1	730
5	Markov state models of biomolecular conformational dynamics. Current Opinion in Structural Biology, 2014, 25, 135-144.	5.7	628
6	Machine Learning for Molecular Simulation. Annual Review of Physical Chemistry, 2020, 71, 361-390.	10.8	456
7	Hierarchical analysis of conformational dynamics in biomolecules: Transition networks of metastable states. Journal of Chemical Physics, 2007, 126, 155102.	3.0	363
8	Spatiotemporal control of endocytosis by phosphatidylinositol-3,4-bisphosphate. Nature, 2013, 499, 233-237.	27.8	362
9	Protein conformational plasticity and complex ligand-binding kinetics explored by atomistic simulations and Markov models. Nature Communications, 2015, 6, 7653.	12.8	344
10	HTMD: High-Throughput Molecular Dynamics for Molecular Discovery. Journal of Chemical Theory and Computation, 2016, 12, 1845-1852.	5.3	343
11	Boltzmann generators: Sampling equilibrium states of many-body systems with deep learning. Science, 2019, 365, .	12.6	332
12	VAMPnets for deep learning of molecular kinetics. Nature Communications, 2018, 9, 5.	12.8	330
13	Machine Learning of Coarse-Grained Molecular Dynamics Force Fields. ACS Central Science, 2019, 5, 755-767.	11.3	306
14	Complete protein–protein association kinetics in atomic detail revealed by molecular dynamics simulations and Markov modelling. Nature Chemistry, 2017, 9, 1005-1011.	13.6	304
15	Learning continuous and data-driven molecular descriptors by translating equivalent chemical representations. Chemical Science, 2019, 10, 1692-1701.	7.4	293
16	Time-lagged autoencoders: Deep learning of slow collective variables for molecular kinetics. Journal of Chemical Physics, 2018, 148, 241703.	3.0	283
17	Crystal structure of nucleotide-free dynamin. Nature, 2011, 477, 556-560.	27.8	277
18	Deep-neural-network solution of the electronic Schrödinger equation. Nature Chemistry, 2020, 12, 891-897.	13.6	272

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19	Variational Approach to Molecular Kinetics. Journal of Chemical Theory and Computation, 2014, 10, 1739-1752.	5.3	256
20	Camostat mesylate inhibits SARS-CoV-2 activation by TMPRSS2-related proteases and its metabolite GBPA exerts antiviral activity. EBioMedicine, 2021, 65, 103255.	6.1	256
21	A Variational Approach to Modeling Slow Processes in Stochastic Dynamical Systems. Multiscale Modeling and Simulation, 2013, 11, 635-655.	1.6	249
22	Data-Driven Model Reduction and Transfer Operator Approximation. Journal of Nonlinear Science, 2018, 28, 985-1010.	2.1	192
23	Markov state models based on milestoning. Journal of Chemical Physics, 2011, 134, 204105.	3.0	184
24	Unsupervised Learning Methods for Molecular Simulation Data. Chemical Reviews, 2021, 121, 9722-9758.	47.7	182
25	Kinetic Distance and Kinetic Maps from Molecular Dynamics Simulation. Journal of Chemical Theory and Computation, 2015, 11, 5002-5011.	5.3	173
26	Multiensemble Markov models of molecular thermodynamics and kinetics. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, E3221-30.	7.1	173
27	On the Approximation Quality of Markov State Models. Multiscale Modeling and Simulation, 2010, 8, 1154-1177.	1.6	160
28	Variational Approach for Learning Markov Processes from Time Series Data. Journal of Nonlinear Science, 2020, 30, 23-66.	2.1	156
29	Projected and hidden Markov models for calculating kinetics and metastable states of complex molecules. Journal of Chemical Physics, 2013, 139, 184114.	3.0	144
30	Efficient multi-objective molecular optimization in a continuous latent space. Chemical Science, 2019, 10, 8016-8024.	7.4	143
31	Protein-peptide association kinetics beyond the seconds timescale from atomistic simulations. Nature Communications, 2017, 8, 1095.	12.8	137
32	EMMA: A Software Package for Markov Model Building and Analysis. Journal of Chemical Theory and Computation, 2012, 8, 2223-2238.	5.3	136
33	Probability distributions of molecular observables computed from Markov models. Journal of Chemical Physics, 2008, 128, 244103.	3.0	123
34	ReaDDy - A Software for Particle-Based Reaction-Diffusion Dynamics in Crowded Cellular Environments. PLoS ONE, 2013, 8, e74261.	2.5	117
35	Collective variables for the study of long-time kinetics from molecular trajectories: theory and methods. Current Opinion in Structural Biology, 2017, 43, 141-147.	5.7	116
36	Machine learning for protein folding and dynamics. Current Opinion in Structural Biology, 2020, 60, 77-84.	5.7	116

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37	Crystal structure of the dynamin tetramer. Nature, 2015, 525, 404-408.	27.8	115
38	Probing molecular kinetics with Markov models: metastable states, transition pathways and spectroscopic observables. Physical Chemistry Chemical Physics, 2011, 13, 16912.	2.8	106
39	Dynamical fingerprints for probing individual relaxation processes in biomolecular dynamics with simulations and kinetic experiments. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 4822-4827.	7.1	105
40	Higher-Order Architecture of Rhodopsin in Intact Photoreceptors and Its Implication for Phototransduction Kinetics. Structure, 2015, 23, 628-638.	3.3	105
41	Coarse graining molecular dynamics with graph neural networks. Journal of Chemical Physics, 2020, 153, 194101.	3.0	103
42	Estimation and uncertainty of reversible Markov models. Journal of Chemical Physics, 2015, 143, 174101.	3.0	102
43	Lipid-mediated PX-BAR domain recruitment couples local membrane constriction to endocytic vesicle fission. Nature Communications, 2017, 8, 15873.	12.8	101
44	TorchMD: A Deep Learning Framework for Molecular Simulations. Journal of Chemical Theory and Computation, 2021, 17, 2355-2363.	5.3	101
45	Variational Koopman models: Slow collective variables and molecular kinetics from short off-equilibrium simulations. Journal of Chemical Physics, 2017, 146, 154104.	3.0	100
46	Nanoscopic compartmentalization of membrane protein motion at the axon initial segment. Journal of Cell Biology, 2016, 215, 37-46.	5.2	99
47	Combining experimental and simulation data of molecular processes via augmented Markov models. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 8265-8270.	7.1	93
48	Kinetic characterization of the critical step in HIV-1 protease maturation. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 20449-20454.	7.1	92
49	Transition Networks for the Comprehensive Characterization of Complex Conformational Change in Proteins. Journal of Chemical Theory and Computation, 2006, 2, 840-857.	5.3	88
50	Structure and assembly of the mitochondrial membrane remodelling GTPase Mgm1. Nature, 2019, 571, 429-433.	27.8	86
51	Complex RNA Folding Kinetics Revealed by Single-Molecule FRET and Hidden Markov Models. Journal of the American Chemical Society, 2014, 136, 4534-4543.	13.7	84
52	Reactive SINDy: Discovering governing reactions from concentration data. Journal of Chemical Physics, 2019, 150, 025101.	3.0	84
53	Simulation tools for particle-based reaction-diffusion dynamics in continuous space. BMC Biophysics, 2014, 7, 11.	4.4	74
54	Statistically optimal analysis of state-discretized trajectory data from multiple thermodynamic states. Journal of Chemical Physics, 2014, 141, 214106.	3.0	73

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55	Alpha 1 Antitrypsin is an Inhibitor of the SARS-CoV-2–Priming Protease TMPRSS2. Pathogens and Immunity, 2021, 6, 55-74.	3.1	73
56	Dynamic properties of force fields. Journal of Chemical Physics, 2015, 142, 084101.	3.0	70
57	Roadmap on Machine learning in electronic structure. Electronic Structure, 2022, 4, 023004.	2.8	69
58	Molecular mechanism of inhibiting the SARS-CoV-2 cell entry facilitator TMPRSS2 with camostat and nafamostat. Chemical Science, 2021, 12, 983-992.	7.4	66
59	Dynamical Organization of Syntaxin-1A at the Presynaptic Active Zone. PLoS Computational Biology, 2015, 11, e1004407.	3.2	65
60	Mechanisms of Protein-Ligand Association and Its Modulation by Protein Mutations. Biophysical Journal, 2011, 100, 701-710.	0.5	62
61	ReaDDy 2: Fast and flexible software framework for interacting-particle reaction dynamics. PLoS Computational Biology, 2019, 15, e1006830.	3.2	59
62	Hierarchical Time-Lagged Independent Component Analysis: Computing Slow Modes and Reaction Coordinates for Large Molecular Systems. Journal of Chemical Theory and Computation, 2016, 12, 6118-6129.	5.3	57
63	Identifying optimal cycles in quantum thermal machines with reinforcement-learning. Npj Quantum Information, 2022, 8, .	6.7	57
64	Dynamical reweighting: Improved estimates of dynamical properties from simulations at multiple temperatures. Journal of Chemical Physics, 2011, 134, 244107.	3.0	55
65	Investigating Molecular Kinetics by Variationally Optimized Diffusion Maps. Journal of Chemical Theory and Computation, 2015, 11, 5947-5960.	5.3	54
66	Variational tensor approach for approximating the rare-event kinetics of macromolecular systems. Journal of Chemical Physics, 2016, 144, 054105.	3.0	53
67	Markov models and dynamical fingerprints: Unraveling the complexity of molecular kinetics. Chemical Physics, 2012, 396, 92-107.	1.9	52
68	Markov Models of Molecular Kinetics. Journal of Chemical Physics, 2019, 151, 190401.	3.0	52
69	Markov state models from short non-equilibrium simulations–Analysis and correction of estimation bias. Journal of Chemical Physics, 2017, 146, .	3.0	51
70	Commute Maps: Separating Slowly Mixing Molecular Configurations for Kinetic Modeling. Journal of Chemical Theory and Computation, 2016, 12, 5620-5630.	5.3	47
71	Optimal use of data in parallel tempering simulations for the construction of discrete-state Markov models of biomolecular dynamics. Journal of Chemical Physics, 2011, 134, 244108.	3.0	46
72	Variational selection of features for molecular kinetics. Journal of Chemical Physics, 2019, 150, 194108.	3.0	46

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73	OpenPathSampling: A Python Framework for Path Sampling Simulations. 1. Basics. Journal of Chemical Theory and Computation, 2019, 15, 813-836.	5.3	45
74	Introduction to Markov state modeling with the PyEMMA software [Article v1.0]. Living Journal of Computational Molecular Science, 2019, 1, .	6.4	45
75	Data-based parameter estimation of generalized multidimensional Langevin processes. Physical Review E, 2007, 76, 016706.	2.1	43
76	Targeted Adversarial Learning Optimized Sampling. Journal of Physical Chemistry Letters, 2019, 10, 5791-5797.	4.6	41
77	Dynamically Driven Allostery in MHC Proteins: Peptide-Dependent Tuning of Class I MHC Global Flexibility. Frontiers in Immunology, 2019, 10, 966.	4.8	41
78	Estimating the sampling error: Distribution of transition matrices and functions of transition matrices for given trajectory data. Physical Review E, 2009, 80, 021106.	2.1	40
79	MHC class II complexes sample intermediate states along the peptide exchange pathway. Nature Communications, 2016, 7, 13224.	12.8	40
80	Single event visualization of unconventional secretion of FGF2. Journal of Cell Biology, 2019, 218, 683-699.	5.2	39
81	Probability distributions of molecular observables computed from Markov models. II. Uncertainties in observables and their time-evolution. Journal of Chemical Physics, 2010, 133, 105102.	3.0	38
82	Explicit Spatiotemporal Simulation of Receptor-G Protein Coupling in Rod Cell Disk Membranes. Biophysical Journal, 2014, 107, 1042-1053.	0.5	38
83	Ensemble learning of coarse-grained molecular dynamics force fields with a kernel approach. Journal of Chemical Physics, 2020, 152, 194106.	3.0	38
84	Deeptime: a Python library for machine learning dynamical models from time series data. Machine Learning: Science and Technology, 2022, 3, 015009.	5.0	37
85	Shedding Light on the Dock–"Lock Mechanism in Amyloid Fibril Growth Using Markov State Models. Journal of Physical Chemistry Letters, 2015, 6, 1076-1081.	4.6	35
86	Mechanistic Models of Chemical Exchange Induced Relaxation in Protein NMR. Journal of the American Chemical Society, 2017, 139, 200-210.	13.7	35
87	Machine learning implicit solvation for molecular dynamics. Journal of Chemical Physics, 2021, 155, 084101.	3.0	35
88	Automated computation of low-energy pathways for complex rearrangements in proteins: Application to the conformational switch of Ras p21. Proteins: Structure, Function and Bioinformatics, 2005, 59, 534-544.	2.6	34
89	It takes two transducins to activate the cGMP-phosphodiesterase 6 in retinal rods. Open Biology, 2018, 8, .	3.6	34
90	OpenPathSampling: A Python Framework for Path Sampling Simulations. 2. Building and Customizing Path Ensembles and Sample Schemes. Journal of Chemical Theory and Computation, 2019, 15, 837-856.	5.3	34

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91	Particle-based membrane model for mesoscopic simulation of cellular dynamics. Journal of Chemical Physics, 2018, 148, 044901.	3.0	33
92	Dynamic graphical models of molecular kinetics. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 15001-15006.	7.1	33
93	Efficient Bayesian estimation of Markov model transition matrices with given stationary distribution. Journal of Chemical Physics, 2013, 138, 164113.	3.0	32
94	What Markov State Models Can and Cannot Do: Correlation versus Path-Based Observables in Protein-Folding Models. Journal of Chemical Theory and Computation, 2021, 17, 3119-3133.	5.3	32
95	The Isomeric Preference of an Atypical Dopamine Transporter Inhibitor Contributes to Its Selection of the Transporter Conformation. ACS Chemical Neuroscience, 2017, 8, 1735-1746.	3.5	31
96	Identification of kinetic order parameters for non-equilibrium dynamics. Journal of Chemical Physics, 2019, 150, 164120.	3.0	31
97	Large-scale simulation of biomembranes incorporating realistic kinetics into coarse-grained models. Nature Communications, 2020, 11, 2951.	12.8	31
98	ReaDDyMM: Fast Interacting Particle Reaction-Diffusion Simulations Using Graphical Processing Units. Biophysical Journal, 2015, 108, 457-461.	0.5	30
99	Neuraldecipher â€" reverse-engineering extended-connectivity fingerprints (ECFPs) to their molecular structures. Chemical Science, 2020, 11, 10378-10389.	7.4	28
100	Multi-body effects in a coarse-grained protein force field. Journal of Chemical Physics, 2021, 154, 164113.	3.0	28
101	Reversible Interacting-Particle Reaction Dynamics. Journal of Physical Chemistry B, 2018, 122, 11240-11250.	2.6	27
102	Predicting the Kinetics of RNA Oligonucleotides Using Markov State Models. Journal of Chemical Theory and Computation, 2017, 13, 926-934.	5.3	26
103	xTRAM: Estimating Equilibrium Expectations from Time-Correlated Simulation Data at Multiple Thermodynamic States. Physical Review X, 2014, 4, .	8.9	25
104	A Basis Set for Peptides for the Variational Approach to Conformational Kinetics. Journal of Chemical Theory and Computation, 2015, 11, 3992-4004.	5.3	25
105	MSM/RD: Coupling Markov state models of molecular kinetics with reaction-diffusion simulations. Journal of Chemical Physics, 2018, 148, 214107.	3.0	25
106	Identifying Conformational-Selection and Induced-Fit Aspects in the Binding-Induced Folding of PMI from Markov State Modeling of Atomistic Simulations. Journal of Physical Chemistry B, 2018, 122, 5649-5656.	2.6	24
107	Rapid Calculation of Molecular Kinetics Using Compressed Sensing. Journal of Chemical Theory and Computation, 2018, 14, 2771-2783.	5.3	24
108	The mechanism of RNA base fraying: Molecular dynamics simulations analyzed with core-set Markov state models. Journal of Chemical Physics, 2019, 150, 154123.	3.0	24

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109	Discovery of a hidden transient state in all bromodomain families. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	24
110	Dynamic neutron scattering from conformational dynamics. I. Theory and Markov models. Journal of Chemical Physics, 2013, 139, 175101.	3.0	22
111	Beating the Millisecond Barrier in Molecular Dynamics Simulations. Biophysical Journal, 2015, 108, 228-229.	0.5	22
112	Collective hydrogen-bond rearrangement dynamics in liquid water. Journal of Chemical Physics, 2018, 149, 244504.	3.0	22
113	Machine Learning for Molecular Dynamics on Long Timescales. Lecture Notes in Physics, 2020, , 331-372.	0.7	22
114	Optimal Identification of Semi-Rigid Domains in Macromolecules from Molecular Dynamics Simulation. PLoS ONE, 2010, 5, e10491.	2.5	21
115	Optimal Estimation of Free Energies and Stationary Densities from Multiple Biased Simulations. Multiscale Modeling and Simulation, 2014, 12, 25-54.	1.6	21
116	Optimal Data-Driven Estimation of Generalized Markov State Models for Non-Equilibrium Dynamics. Computation, 2018, 6, 22.	2.0	20
117	Molecular dynamics simulations data of the twenty encoded amino acids in different force fields. Data in Brief, 2016, 7, 582-590.	1.0	17
118	An efficient multi-scale Green's function reaction dynamics scheme. Journal of Chemical Physics, 2017, 147, 184106.	3.0	17
119	Nanoscale coupling of endocytic pit growth and stability. Science Advances, 2019, 5, eaax5775.	10.3	17
120	Kernel methods for detecting coherent structures in dynamical data. Chaos, 2019, 29, 123112.	2.5	17
121	Spectral Rate Theory for Two-State Kinetics. Physical Review X, 2014, 4, .	8.9	16
122	Projected metastable Markov processes and their estimation with observable operator models. Journal of Chemical Physics, 2015, 143, 144101.	3.0	15
123	Geometrical characterization of T cell receptor binding modes reveals class‐specific binding to maximize access to antigen. Proteins: Structure, Function and Bioinformatics, 2020, 88, 503-513.	2.6	15
124	Gaussian Markov transition models of molecular kinetics. Journal of Chemical Physics, 2015, 142, 084104.	3.0	14
125	Diffusion-influenced reaction rates in the presence of pair interactions. Journal of Chemical Physics, 2019, 151, 164105.	3.0	14
126	Polymer-like Model to Study the Dynamics of Dynamin Filaments on Deformable Membrane Tubes. Biophysical Journal, 2019, 117, 1870-1891.	0.5	13

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127	Convergence to the fixed-node limit in deep variational Monte Carlo. Journal of Chemical Physics, 2021, 154, 124108.	3.0	13
128	Multiscale molecular kinetics by coupling Markov state models and reaction-diffusion dynamics. Journal of Chemical Physics, 2021, 155, 124109.	3.0	13
129	A litmus test for classifying recognition mechanisms of transiently binding proteins. Nature Communications, 2022, 13, .	12.8	13
130	Dynamic neutron scattering from conformational dynamics. II. Application using molecular dynamics simulation and Markov modeling. Journal of Chemical Physics, 2013, 139, 175102.	3.0	12
131	Grand canonical diffusion-influenced reactions: A stochastic theory with applications to multiscale reaction-diffusion simulations. Journal of Chemical Physics, 2018, 149, 044102.	3.0	12
132	Deflation reveals dynamical structure in nondominant reaction coordinates. Journal of Chemical Physics, 2019, 151, .	3.0	12
133	Cyclization and Relaxation Dynamics of Finite-Length Collapsed Self-Avoiding Polymers. Physical Review Letters, 2019, 122, 067801.	7.8	12
134	Coupling of Conformational Switches in Calcium Sensor Unraveled with Local Markov Models and Transfer Entropy. Journal of Chemical Theory and Computation, 2020, 16, 2584-2593.	5.3	12
135	Thermodynamics and Kinetics of Aggregation of Flexible Peripheral Membrane Proteins. Journal of Physical Chemistry Letters, 2021, 12, 10497-10504.	4.6	12
136	Synergistic inhibition of SARS-CoV-2 cell entry by otamixaban and covalent protease inhibitors: pre-clinical assessment of pharmacological and molecular properties. Chemical Science, 2021, 12, 12600-12609.	7.4	11
137	Independent Markov decomposition: Toward modeling kinetics of biomolecular complexes. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	11
138	Progress in deep Markov state modeling: Coarse graining and experimental data restraints. Journal of Chemical Physics, 2021, 155, 214106.	3.0	10
139	Symmetric and antisymmetric kernels for machine learning problems in quantum physics and chemistry. Machine Learning: Science and Technology, 2021, 2, 045016.	5.0	9
140	Parameterized Hypercomplex Graph Neural Networks for Graph Classification. Lecture Notes in Computer Science, 2021, , 204-216.	1.3	9
141	grünifai: interactive multiparameter optimization of molecules in a continuous vector space. Bioinformatics, 2020, 36, 4093-4094.	4.1	7
142	Coupling Particle-Based Reaction-Diffusion Simulations with Reservoirs Mediated by Reaction-Diffusion PDEs. Multiscale Modeling and Simulation, 2021, 19, 1659-1683.	1.6	7
143	A scalable approach to the computation of invariant measures for high-dimensional Markovian systems. Scientific Reports, 2018, 8, 1796.	3.3	6
144	Hydrodynamic coupling for particle-based solvent-free membrane models. Journal of Chemical Physics, 2021, 155, 114108.	3.0	5

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145	Porting Adaptive Ensemble Molecular Dynamics Workflows to the Summit Supercomputer. Lecture Notes in Computer Science, 2019, , 397-417.	1.3	5
146	Neural mode jump Monte Carlo. Journal of Chemical Physics, 2021, 154, 074101.	3.0	4
147	Generating stable molecules using imitation and reinforcement learning. Machine Learning: Science and Technology, 2022, 3, 015008.	5.0	4
148	Response to Comment â€œTransient Complexes between Dark Rhodopsin and Transducin: Circumstantial Evidence or Physiological Necessity?â€•byÂD. Dellâ€™Orco and K.-W. Koch. Biophysical Journal, 2015, 108, 778-779.	0.5	3
149	Computational tools for analysing structural changes in proteins in solution. Applied Bioinformatics, 2003, 2, S11-7.	1.6	0